Electronic supplementary information for

Carbazole and/or triphenylamine-based D-π-D multiarylamino dyes: Synthesis, characterization and photophysical properties

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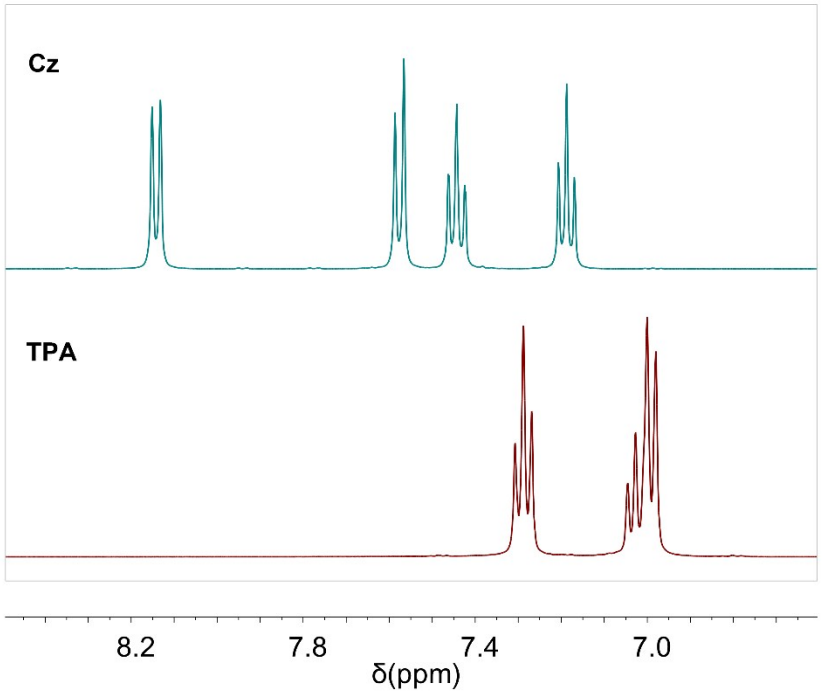


Fig. S1. [1]H NMR spectra of carbazole (**Cz**) and triphenylamine (**TPA**).

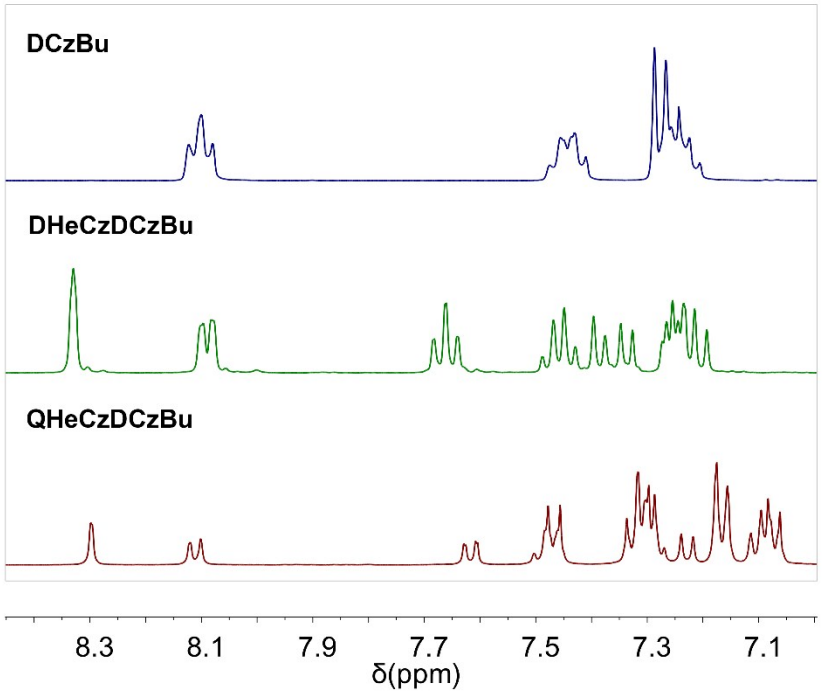


Fig. S2. [1]H NMR spectra of **DCzBu**, **DHeCzDCzBu** and **DTPADCzBu**.

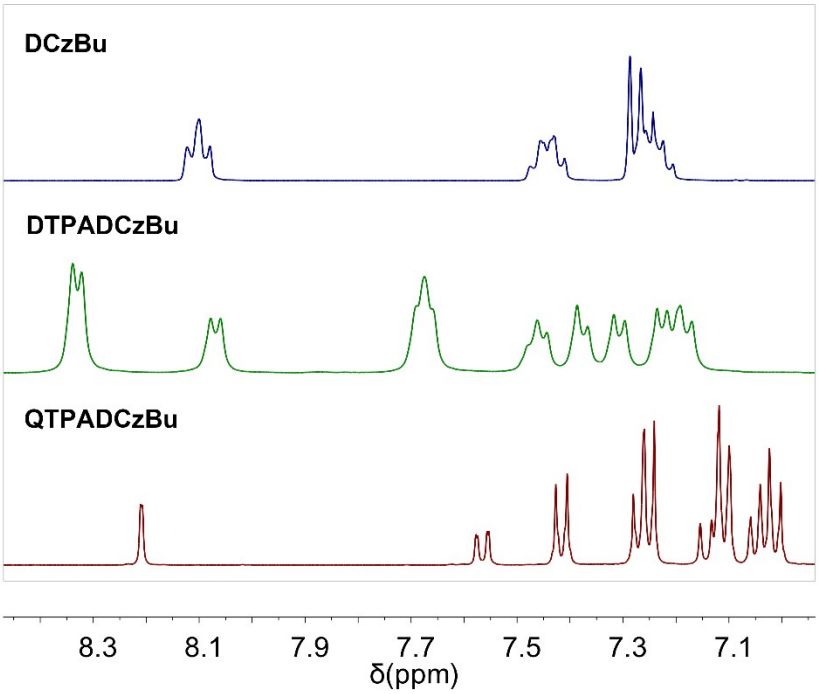


Fig. S3. ^{1}H NMR spectra of **DCzBu**, **QHeCzDCzBu** and **QTPADCzBu**.

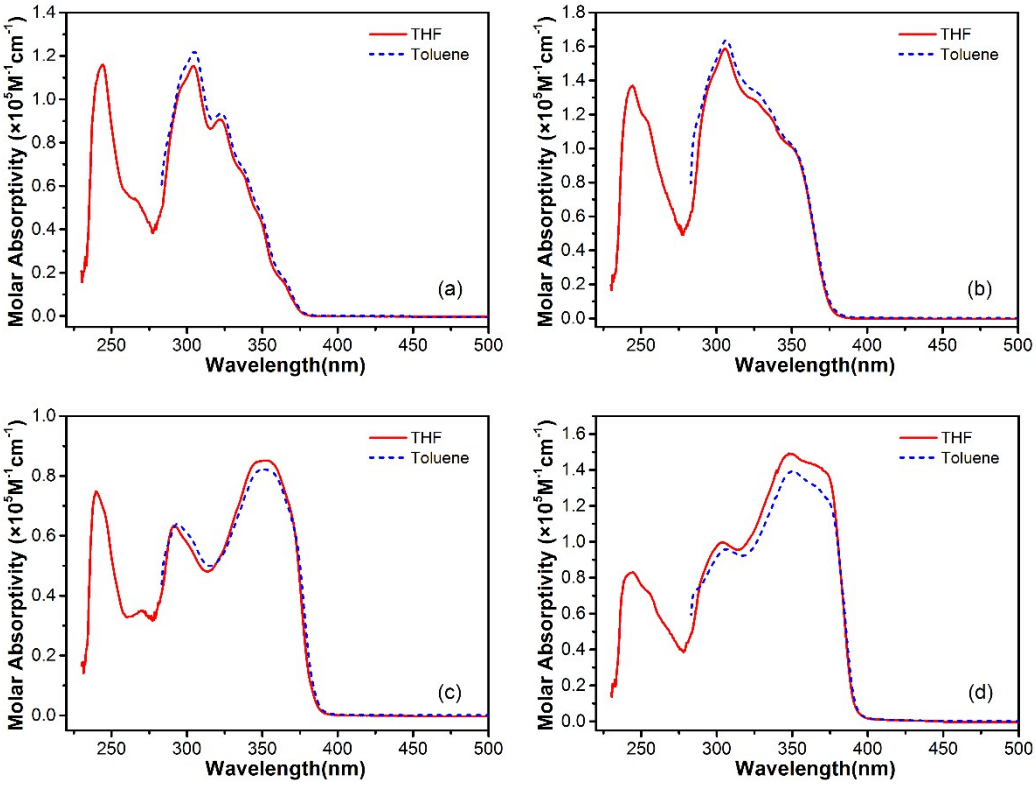


Fig. S4. Comparison of UV-vis spectra in THF and Toluene (1×10^{-5} M) of (a) **DHeCzDCzBu**; (b) **QHeCzDCzBu**; (c) **DTPADCzBu**; (d). **QTPADCzBu**

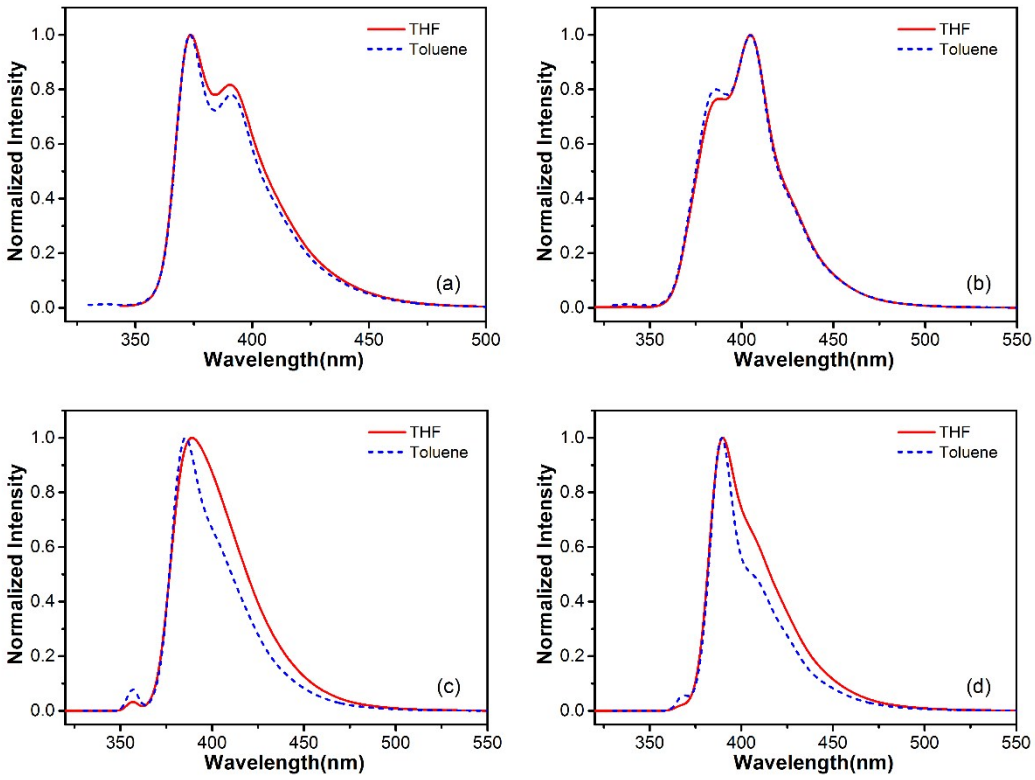


Fig. S5. Comparison of Normalized fluorescence spectra of in THF and Toluene (1×10^{-6} M) (a) **DHeCzDCzBu**; (b) **QHeCzDCzBu**; (c) **DTPADCzBu**; (d). **QTPADCzBu**.

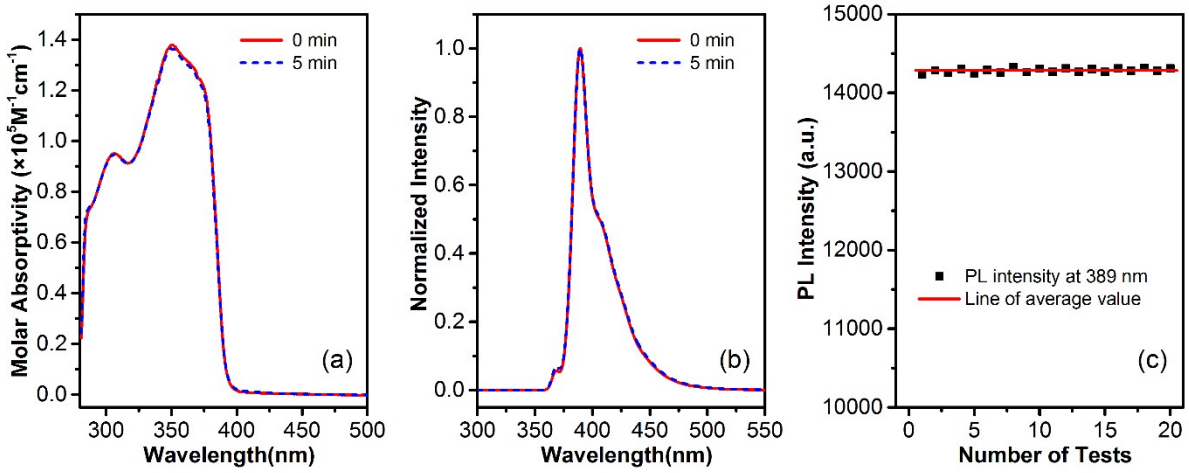


Fig. S6. Comparison of (a) UV-vis spectra and (b) fluorescence spectra of **QTPADCzBu** (1×10^{-5} M) Toluene before and after irradiated by 75 W halogen lamp (I = 10 mW/cm^2) for 5 min; (c) Plots of the intensity of the peak of the emission spectra of **QTPADCzBu** recorded by 20 times.

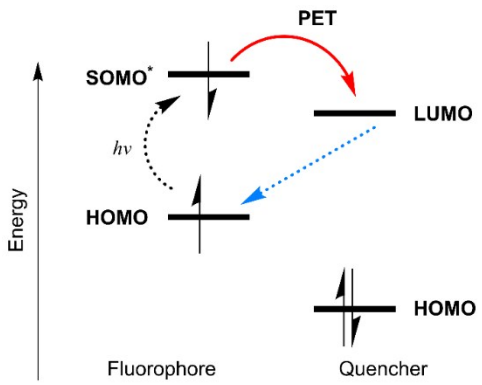


Fig. S7. Energy diagram for photoinduced electron transfer leading to fluorescence quenching.

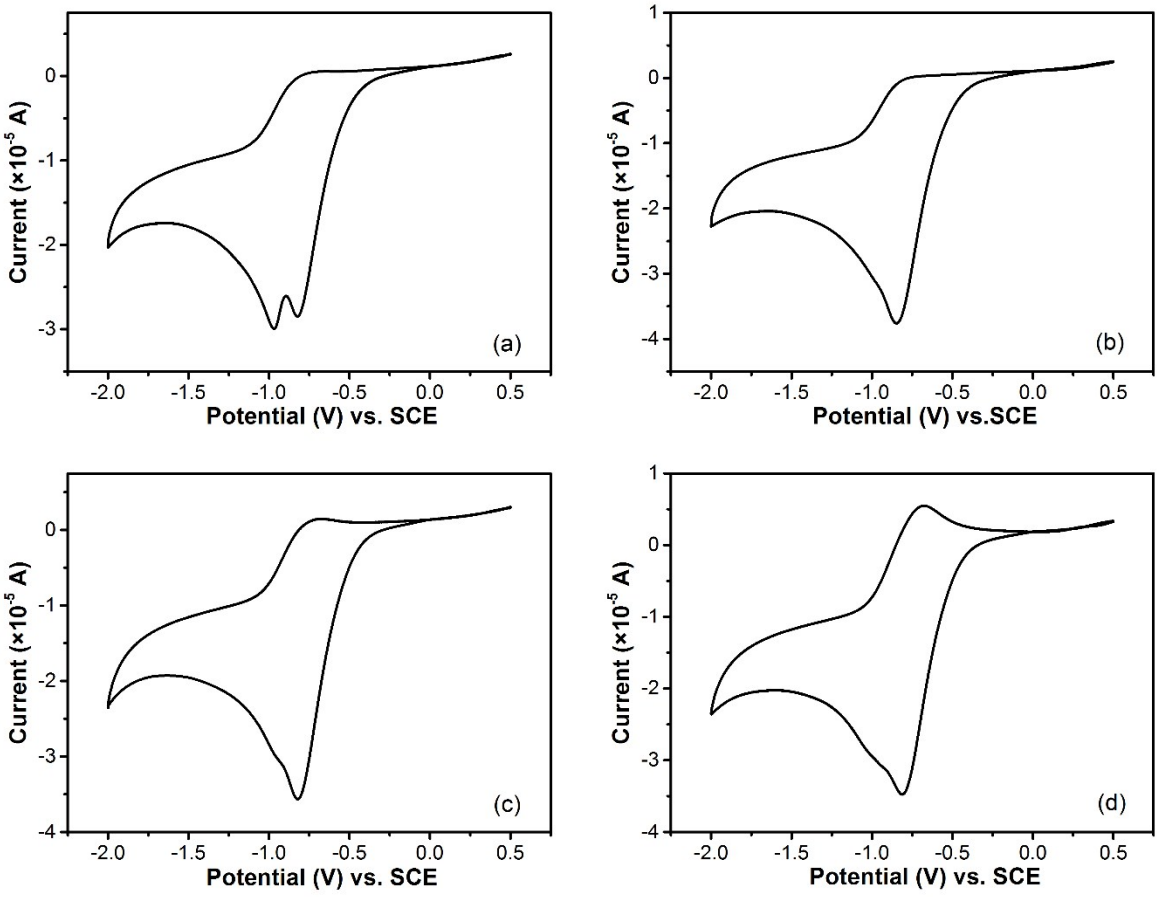


Fig. S8. Cyclic voltammetry curves of (a) **DHeCzDCzBu**; (b) **QHeCzDCzBu**; (c) **DTPADCzBu**; (d). **QTPADCzBu** in DMF (1×10^{-3} M) using 0.1 M tetrabutyl ammonium hexafluorophosphate as the supporting electrolyte, recorded at 100 mV s^{-1} scan speed.

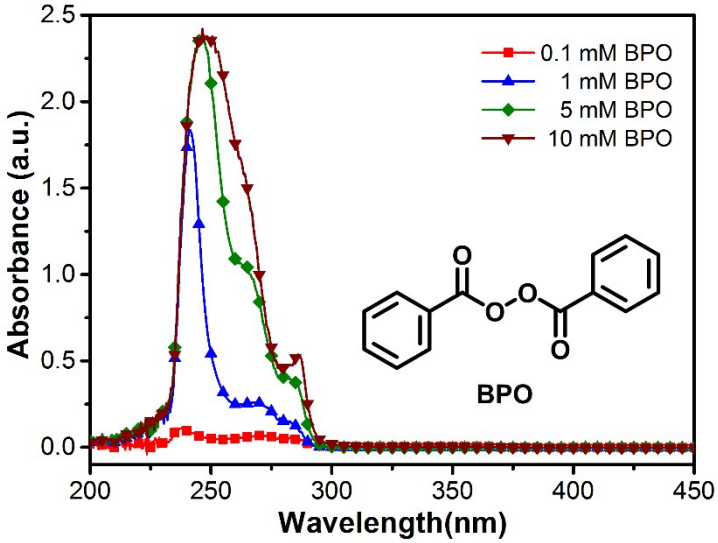
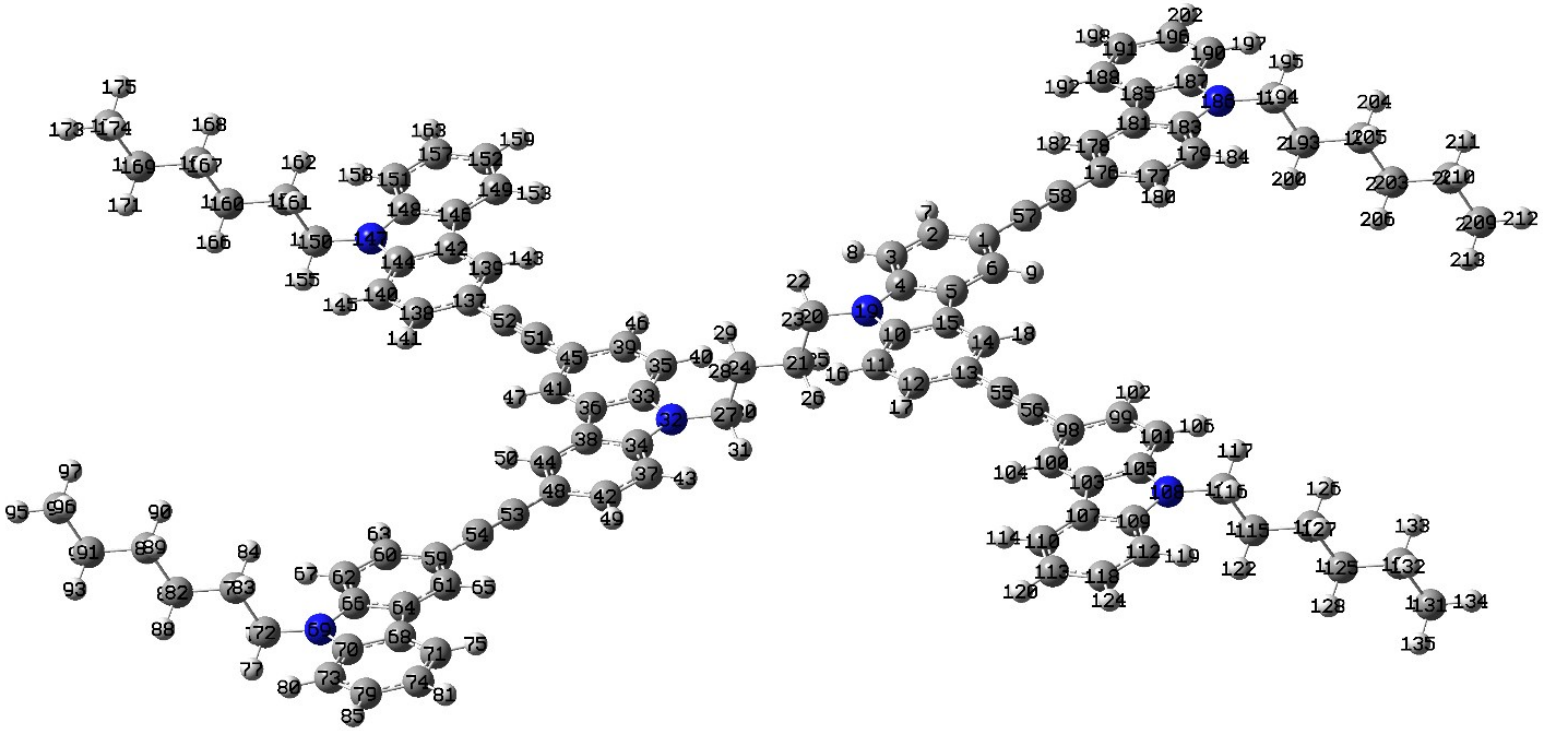


Fig. S9. UV-vis spectra of BPO in THF at different concentrations.

Table S1. The optimized structure and part data of selected bond lengths, angles and dihedral angles of **DHeCzDCzBu**

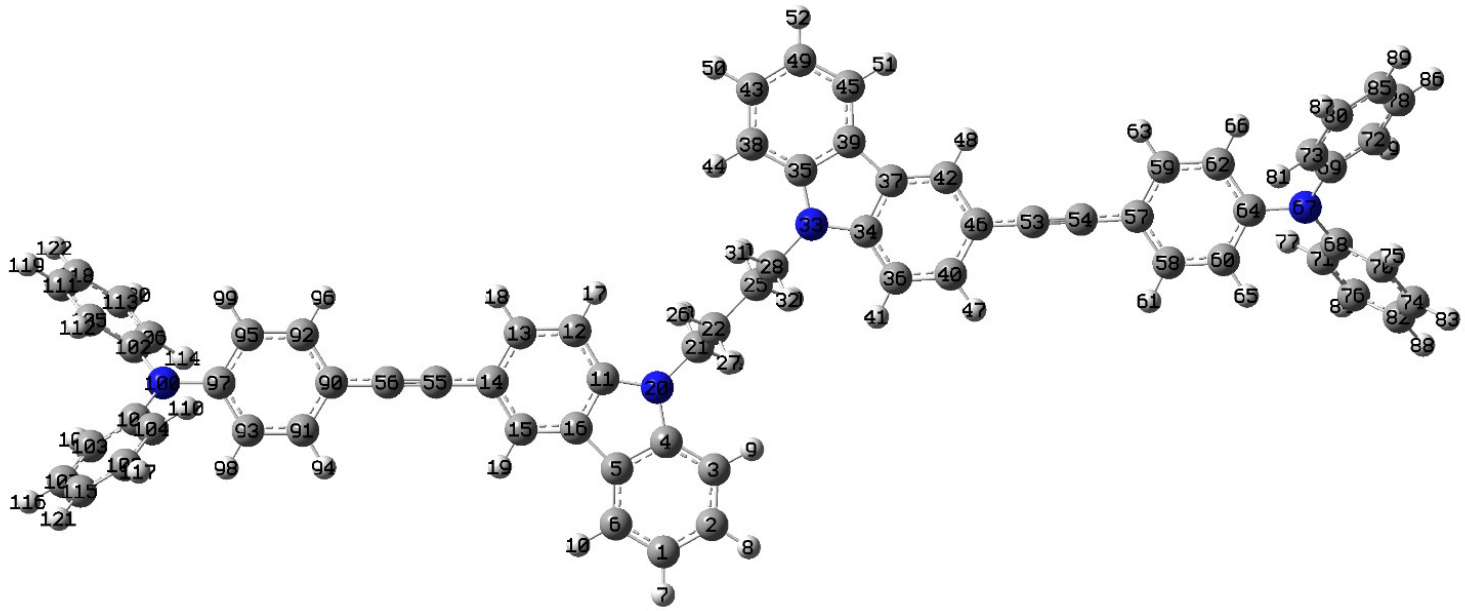
Bond lengths(Å)		**Bond angles**(°)		**Dihedral angle**(°)	
N(20)-C(21)	1.4517	C(4)-N(20)-C(21)	125.63	C(3)-C(4)-N(20)-C(21)	-3.93
C(21)-C(22)	1.5371	N(20)-C(21)-C(22)	113.54	C(4)-N(20)-C(21)-C(22)	-87.61
C(53)-C(54)	1.2173	C(21)-C(22)-C(25)	112.33	C(43)-C(49)-C(96)-C(98)	0.13
N(67)-C(70)	1.4537	N(67)-C(70)-C(74)	113.75	C(64)-N(67)-C(70)-C(74)	87.77

Table S2 The optimized structure and part data of selected bond lengths, angles and dihedral angles of **QHeCzDCzBu**



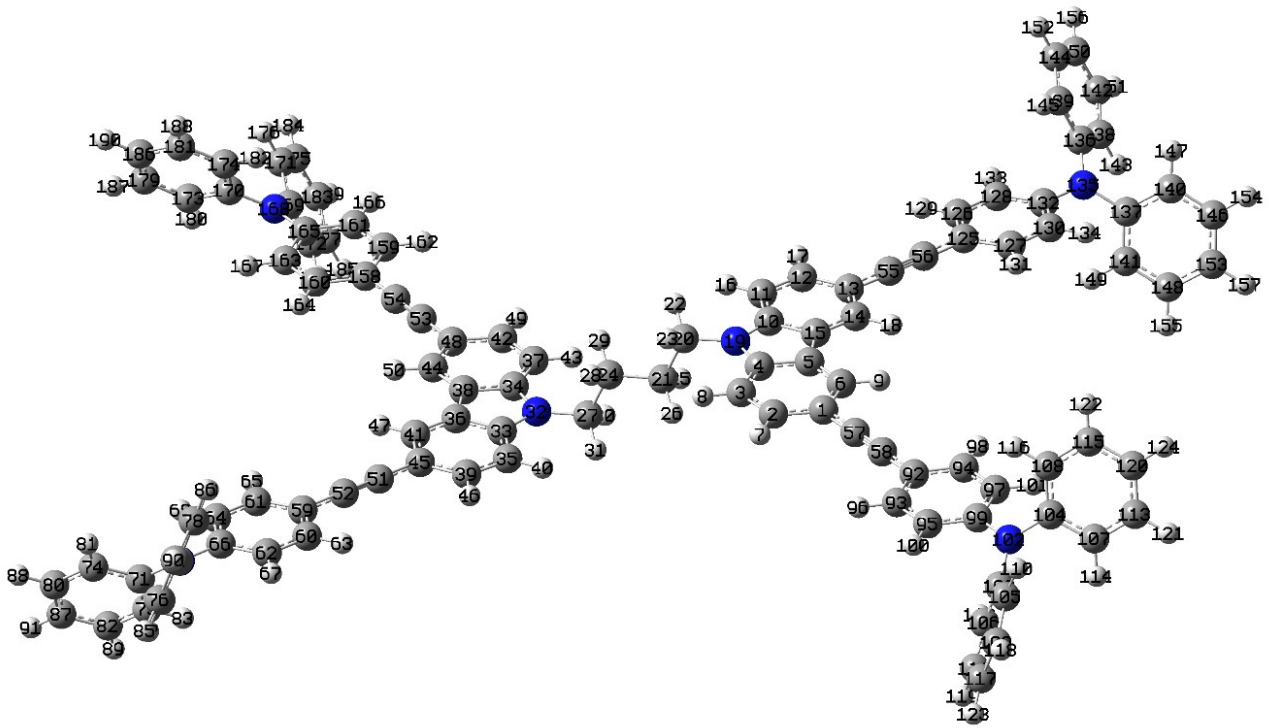
Bond lengths(Å)		**Bond angles**(°)		**Dihedral angle**(°)	
N(19)-C(20)	1.4524	C(4)-N(19)-C(20)	125.60	C(3)-C(4)-N(19)-C(20)	4.27
C(20)-C(21)	1.5368	C(14)-C(13)-C(57)	120.69	C(4)-N(19)-C(20)-C(21)	87.01
C(53)-C(54)	1.2173	N(19)-C(20)-C(21)	113.43	C(14)-C(13)-C(98)-C(99)	2.94
N(69)-C(72)	1.4537	C(66)-N(69)-C(72)	125.69	C(66)-N(69)-N(72)-C(76)	-87.95

Table S3. The optimized structure and part data of selected bond lengths, angles and dihedral angles of **DTPADCzBu**



Bond lengths(Å)		**Bond angles**(°)		**Dihedral angle**(°)	
N(20)-C(21)	1.4519	C(4)-N(20)-C(21)	125.62	C(3)-C(4)-N(20)-C(21)	-4.00
C(21)-C(22)	1.5370	C(13)-C(14)-C(55)	120.01	C(4)-N(20)-C(21)-C(22)	-87.00
C(53)-C(54)	1.2176	N(20)-C(21)-C(22)	113.48	C(13)-C(14)-C(90)-C(92)	0.79
C(64)-N(67)	1.4167	C(64)-N(67)-C(68)	120.26	C(62)-C(64)-N(67)-C(69)	38.65

Table S4. The optimized structure and part data of selected bond lengths, angles and dihedral angles of **QTPADCzBu**



Bond lengths(Å)		**Bond angles**(°)		**Dihedral angle**(°)	
C(27)-N(32)	1.4525	C(4)-N(19)-C(20)	125.71	C(3)-C(4)-N(19)-C(20)	-2.45
C(24)-C(27)	1.5367	C(14)-C(13)-C(55)	120.64	C(4)-N(19)-C(20)-C(21)	-88.34
C(53)-C(54)	1.2175	N(19)-C(20)-C(21)	113.58	C(14)-C(13)-C(125)-C(127)	-5.30
C(66)-N(69)	1.4162	C(66)-N(69)-C(70)	120.20	C(62)-C(66)-N(69)-C(70)	38.03

Table S5. UV-vis absorption data of **DCzBu** and DCzBus in THF and Toluene (1×10^{-5} M)

Compounds	Solvents	λ_1 [a]	ε_1 [b]	λ_2 [a]	ε_2 [b]	λ_3 [a]	ε_3 [b]
DCzBu	THF	239	6.02	262	3.81	294	2.80
	Toluene	-	-	-	-	294	3.01
DHeCzDCzBu	THF	245	11.59	305	11.54	322	9.06
	Toluene	-	-	305	12.21	322	9.35
QHeCzDCzBu	THF	245	13.70	306	15.86	-	-
	Toluene	-	-	306	16.39	-	-
DTPADCzBu	THF	240	7.49	291	6.33	355	8.51
	Toluene	-	-	294	6.41	351	8.23
QTPADCzBu	THF	245	8.30	305	9.96	348	14.92
	Toluene	-	-	307	9.59	351	13.95

[a] Wavelength (unit: nm) and [b] Molar absorption coefficient (unit: 10^4 $M^{-1}\cdot cm^{-1}$) of *i*-th maximum absorption peak.

Table S6. Fluorescence data of **DCzBu** and DCzBus in THF and Toluene (1×10^{-6} M)

Compounds	Data measured in THF			Data measured in Toluene		
	Ex_{max} [a] (nm)	Em_{max} [b] (nm)	Φ [d]	Ex_{max} [a] (nm)	Em_{max} [b] (nm)	Φ [d]
DCzBu	293	350 (366) [c]	0.16	293	351 (367) [c]	0.23
DHeCzDCzBu	304	374 (391) [c]	0.25	305	373 (391) [c]	0.36
QHeCzDCzBu	306	405 (388) [c]	0.24	306	405 (387) [c]	0.32
DTPADCzBu	355	389	0.57	355	386	0.60
QTPADCzBu	366	390	0.58	366	390	0.64

Maximum [a] excitation and [b] emission wavelength; [c] Wavelength of shoulder peak of maximum emission peak; [d] Quantum yield of fluorescence, relative to quinine sulfate (0.1 M H_2SO_4 solution).

Table S7. The calculation outcomes of the TPA cross-sections of DCzBus under different excitation laser wavelengths

Wavelength (nm)	σ_{TPA} (GM)			
	DHeCzDCzBu	**QHeCzDCzBu**	**DTPADCzBu**	**QTPADCzBu**
720	8.88	25.07	42.38	107.68
730	10.25	24.69	42.71	112.68
740	5.90	18.48	35.11	93.40
750	3.28	15.07	32.78	94.36
760	1.30	8.84	22.25	82.27
770		2.81	8.53	47.33
780		0.78	2.06	17.12
790			1.03	7.47
800				1.82
810				1.89